The critical point ratio for some $d = 2$ classical models

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ABSTRACT. The universal critical point ratio of the square of the second moment of the order parameter to its fourth moment, denoted as Q, is exploited to determine the position of the critical Ising transition lines in the phase diagram of the Ashkin-Teller (AT) model on the square lattice. A leading-order expansion of the Q ratio in the presence of a non-vanishing thermal field is found from finite-size scaling and the corresponding expression is fitted to the accurate perturbative transfer-matrix data for the $L \times L$ square clusters with $L \leq 9$. The same method is used to determine the critical Ising transition line on the phase diagram of the Blume-Capel (BC) model ($L \leq 11$). We have also calculated the Q ratio for the $q = 3$ Potts model in the critical point. The previously predicted scaling relation for this universality class is confirmed by our results for $L \leq 12$.

1 Ashkin-Teller model

The AT model has first been proposed as a model of a four-component alloy [1]. It has attracted a lot of theoretical interest for years because it is a simple and non-trivial generalisation of the Ising and four-state Potts models. Fan [2] has shown that the hamiltonian of the AT model can also be written with two Ising variables ($S = \pm 1, \sigma = \pm 1$) located at each site of the lattice, and in the presence of a magnetic field it has the form:

$$\mathcal{H} = -\sum_{<i,j>} (J_1 S_i S_j + J_2 \sigma_i \sigma_j + J_4 S_i \sigma_i S_j \sigma_j + J_0) - h \sum_{i=1}^{N} S_i \sigma_i \tag{1}$$

Herein we consider only nearest neighbour pair interactions on the simple square lattice consisting of $N = L^2$ sites with periodic boundary conditions and we assume that $J_1 = J_2$ (isotropic case).

Wagner [3] has shown that the AT model is equivalent to the alternated eight vertex model, which has not been solved exactly. Only one critical line in the phase diagram of the isotropic AT model is known exactly thanks to the duality relation found by Fan [4]. For this reason many approximate approaches have been applied for constructing the complete phase diagram: the mean field theory (MFA) [5, 6], mean-field renormalisation group (MFRG) [7], renormalisation group (RG) [8], and Monte Carlo renormalisation group (MCRG) [9]. It is the aim of this paper to establish an accurate location of the remaining critical lines.

In our approach we exploit finite-size scaling for the ratio of the square of the second moment to the fourth moment of the order parameter M:

$$Q_L = \frac{< M^2 >_L^2}{< M^4 >_L} , \tag{2}$$

where $< ... >$ means thermal average and the index L indicates the linear size of the system $(L \times L)$. In the limit $L \to \infty$ this ratio becomes universal in the critical point [10] and is denoted Q hereafter. Three not exactly known critical lines of the isotropic AT model are believed to belong to the Ising universality class [5, 11]. Here it is assumed that these lines correspond to Ising-like continuous transitions with the order parameter $M = \sum_{i=1}^{N} S_i \sigma_i$. A scaling formula for Q_L can be derived starting from the finite-size scaling relation for the singular part of the free energy for the square Ising model [12].

$$F^{(S)}(g_t, g_h, L^{-1}) = A(g_t L) \ln L + B(g_t L, g_h L^{y_h}) \tag{3}$$

where A and B are unknown amplitudes, g_t, g_h are nonlinear scaling fields and y_h is the magnetic critical exponent. The nonlinear scaling fields g_t and g_h can be expanded in terms of the corresponding linear thermal and magnetic scaling fields t and h.

Taking into account the relations between the magnetization moments in Eq. (2) and the corresponding derivatives of the free energy [12] we have calculated the scaling expansion for $Q_L(t, h = 0)$ to the leading order in t and up to L^{3-4y_h}:

$$Q_L(t) = Q_L(0) + \left.\frac{\partial Q_L(t)}{\partial t}\right|_{t=0} t + ... \tag{4}$$

The zeroth order term $Q_L(0)$ was evaluated previously [12] and the first order term is of the form

$$\begin{aligned} \left.\frac{\partial Q_L(t)}{\partial t}\right|_{t=0} &= \alpha_1 L + \alpha_2 + \alpha_3 L^{3-2y_h} + (\alpha_4 + \alpha_5 \ln L) L^{2-2y_h} + \alpha_6 L^{5-4y_h} + \\ &+ (\alpha_7 + \alpha_8 \ln L) L^{1-2y_h} + (\alpha_9 + \alpha_{10} \ln L) L^{4-4y_h} + \alpha_{11} L^{-2y_h} + \\ &+ (\alpha_{12} + \alpha_{13} \ln L) L^{7-6y_h} + (\alpha_{14} + \alpha_{15} \ln L + \alpha_{16} \ln^2 L) L^{3-4y_h} + ... , \end{aligned} \tag{5}$$

where α_i ($i = 1, ...16$) are unknown amplitudes. In our work we consider only the first three terms in the expansion (5), but for some future Monte Carlo applications the higher order terms in $1/L$ might be important.

We have calculated the $Q_L(t)$ ratio exploiting the transfer matrix (TM) technique which for the Ising model was explained in [12]. Our system consists of L columns containing L sites. Spins from the jth column are denoted by

$$\vec{\Sigma}_j = (S_{j1}, \sigma_{j1}, S_{j2}, \sigma_{j2}, ..., S_{jL}, \sigma_{jL})$$

so that

$$Z = \sum_{\vec{\Sigma}_1, \vec{\Sigma}_2, ..., \vec{\Sigma}_L} \exp(-\beta H(\vec{\Sigma}_1, ..., \vec{\Sigma}_L)) = \mathrm{Tr}\, \mathbf{T}^L \ , \tag{6}$$

where $\mathbf{T}$ is a $4^L \times 4^L$ transfer matrix. This can be split into the product $\mathbf{T} = \mathbf{T}_h \mathbf{T}_v$ of a diagonal matrix $\mathbf{T}_v$ and a non-diagonal matrix $\mathbf{T}_h$ containing the intra- and the inter-column interactions respectively. They are defined as follows

$$\mathbf{T}_v(\vec{\Sigma}_k, \vec{\Sigma}_l) = \delta_{\vec{\Sigma}_k, \vec{\Sigma}_l} \exp\left(\sum_{i=1}^{N} (K_2 S_{k,i} S_{k,i+1} + K_2 \sigma_{k,i} \sigma_{k,i+1} + \right. \tag{7}$$

$$\left. + K_4 S_{k,i} \sigma_{k,i} S_{k,i+1} \sigma_{k,i+1} + H S_{k,i} \sigma_{k,i})\right)$$

$$\mathbf{T}_h(\vec{\Sigma}_k, \vec{\Sigma}_l) = \exp\left(\sum_{i=1}^{N} (K_2 S_{k,i} S_{l,i} + K_2 \sigma_{k,i} \sigma_{l,i} + K_4 S_{k,i} \sigma_{k,i} S_{l,i} \sigma_{l,i})\right) , \tag{8}$$

where , $\beta = \frac{1}{k_B T}$, $K_i = J_i \beta$ ($i = 1, 2, 4$) and $H = \beta h$. The latter matrix can be expressed as a product of sparse matrices which facilitates the numerical calculations.

The averages in Eq. (2) can be expressed in terms of the corresponding coefficients Z_k [12] in the expansion of the field dependent partition function $Z(h) = \sum_{k=0}^{\infty} Z_k \frac{h^k}{k!}$. follows: The coefficients Z_k can then be calculated from Eq. (6) by multiplying the base vectors by matrices $\mathbf{T}_v$ and $\mathbf{T}_h$ in such a manner that the terms in the same power of h are kept separately [12].

At first we calculate the amplitudes α_i ($i \leq 5$) from Eqs (4) and (5) with known values $Q_L(0)$. In the limit $K_2 = 0$, i.e. the Ising model in $S\sigma$, $K_{4c} = K_c = \frac{1}{2}\ln(1 + \sqrt{2})$ and in this case we have only one coupling constant (K_4). Thus we can write the reduced temperature in the form:

$$t = \frac{K_{4c} - K_4}{K_4} \ . \tag{9}$$

Selecting different values of the scaling field t we can solve the set of linear algebraic equations for α_i. For the ferromagnetic coupling K_4 we consider the system sizes $L = 2, 3, ..., 9$ whereas for the antiferromagnetic one only the even values $L = 2, 4, 6, 8$ are considered, so that we can evaluate the coefficients α_i up to $i = 5$ or $i = 3$, respectively.

Having fixed $K_2 \neq 0$ and knowing the α_i $(i \leq 3)$ and $Q_L(0)$, we have calculated (by TM method) $Q_L(K_2, K_4)$ for a number of couplings K_4. This enables a determination of the corresponding t values from Eqs (4) and (5). Then knowing t we can easily obtain K_{4c} from Eq. (9) and K_{2c} from a similar equation, but written for K_2. The estimates K_{4c} and K_{2c} are very stable if we find $t \in < 10^{-7}, 10^{-4} >$.

The exactly known critical curve with continuously varying critical exponents [11] is terminated in the 4-state Potts point where it bifurcates. In the vicinity of this point the convergence of our results is diminished and the estimates of K_{4c} become size dependent. This size dependence is illustrated in Fig. 1.

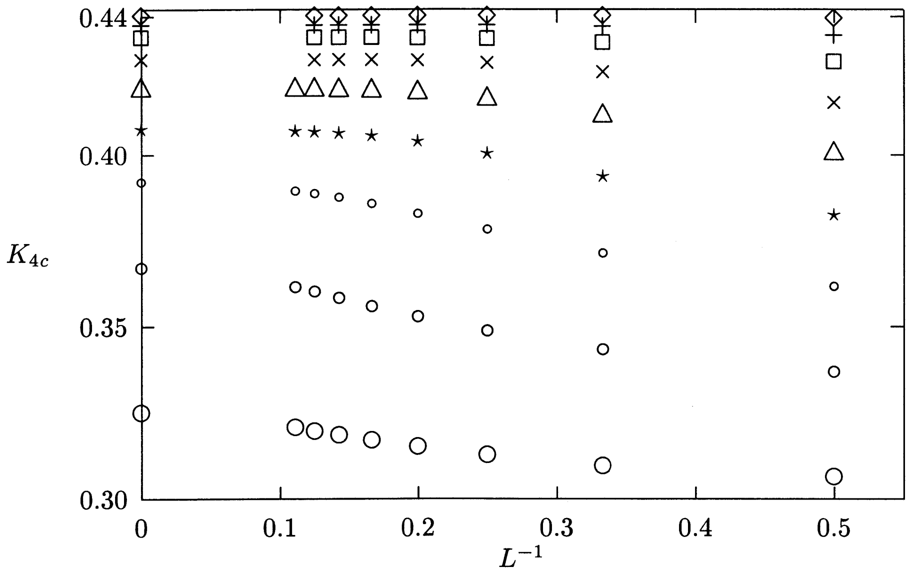

Figure 1: The L-dependence of the critical values of the parameter K_{4c}. The points on the vertical axis are the extrapolated values.

Due to the limited number of system sizes available in our calculations we do not try to include any corrections to scaling and we simply extrapolate our data. Because of the character of the size dependence as a final result we take the average of the extrapolated value and the result for the largest system. They are shown on the ordinate axis in Fig. 1. (We estimate the accuracy of the results obtained in such a way as half the difference between the lineary extrapolated value and the result for the largest system.) Such a strong size dependence does not occur for the antiferromagnetic couplings, since there is no Potts point in this case.

Our final results represented by open circles connected by thin continuous lines are shown in Fig. 2 and they are compared with other results and predictions.

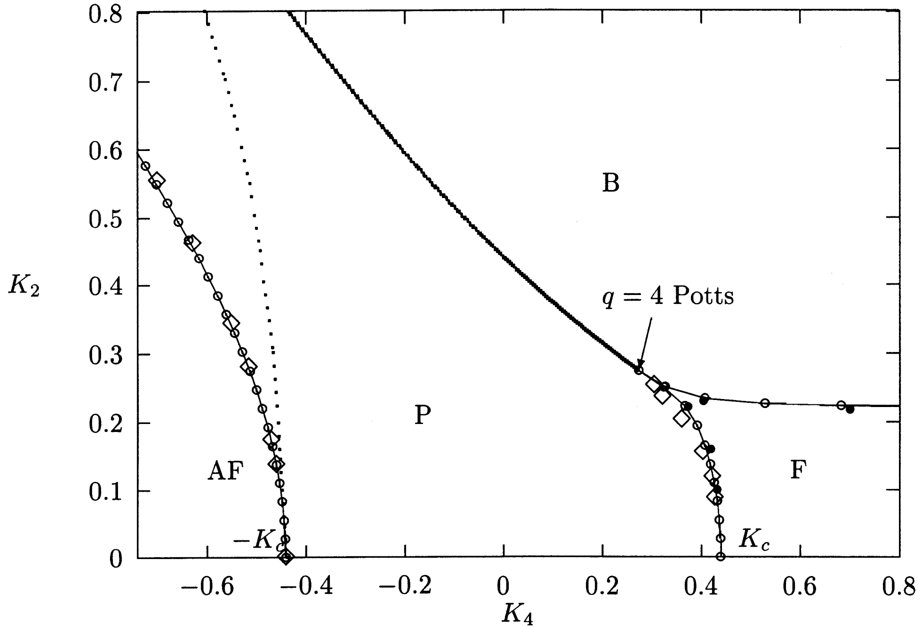

Figure 2: Phase diagram of the AT model in two dimensions. The solid bold line represents the exactly known critical line, which terminates at the 4-state Potts point. Empty circles with continuous lines describe our results. The solid circles display MCRG results , the dotted line is drawn after Baxter and diamonds are the transfer matrix results combined with conformal invariance.

The numerical uncertainties do not exceed the size of the symbol. The curve plotted by the bold line represents the part of the phase diagram found exactly by Baxter [11]. It separates the Baxter phase B from the paramagnetic phase P. The ferromagnetic and antiferromagentic phases with non-vanishing order parameter M are denoted by the labels F and AF, respectively.

In the ferromagnetic region $K_4 > 0$ we have only calculated the curve joining the 4-state Potts point to the pure Ising point K_c at $K_2 = 0$. The second branch follows from the corresponding duality relation [5, 11]. In the boundary between AF and P phases we plot with the dotted line the approximate curve as given by Baxter [11] and in the ferromagnetic region we also include the MCRG results marked by filled circles.

As can be seen (Fig. 2), our results are in good agreement with the MCRG [9] approach, but they are quite different from Baxter's predictions [11] in the antiferromagnetic region. For the boundary between AF and P phases, our results coincide with those obtained by Mazzeo *et al.* [13]. These authors actually in-

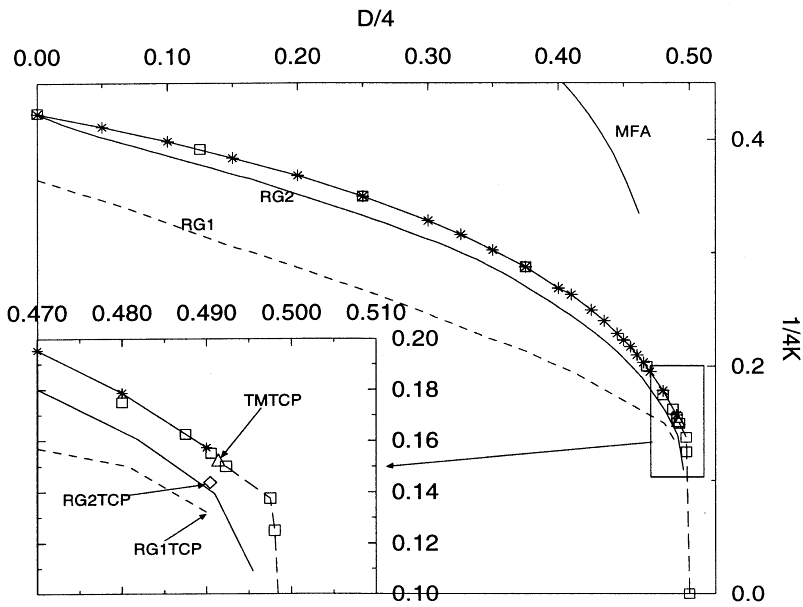

Figure 3: The phase diagram of the Blume-Capel model ($D = \Delta/K$). Our results are drawn with stars connected by lines. RG1 and RG2 are lines of continuous transition predicted by two different RG approaches [17]. Earlier results obtained by TM method [19] are drawn with squares and a long dashed line connects points which belong to the first order transiton line.

vestigated the six vertex model with the transfer matrix technique in combination with conformal invariance arguments; their results can be mapped onto the results for the P-phase boundaries and they are shown in Fig. 2.

As to our accuracy: near the ferromagnetic Ising point it is around $2 * 10^{-6}$ and in the neighbourhood of the Potts point it decreases down to about $3 * 10^{-2}$. The accuracy in the antiferromagnetic region is even better: near the Ising point it reaches $5 * 10^{-8}$ and for the highest point in the phase diagram in Fig. 2 it decreases to $3 * 10^{-3}$.

2 Blume-Capel model

The same method was used to determine the position of the critical Ising transition line in the phase diagram of the $d = 2$ BC model (on the square lattice $L \times L$), with reduced hamiltonian:

$$\beta\mathcal{H} = -K \sum_{<i,j>} S_i S_j + \Delta \sum_i S_i^2, \tag{10}$$

where $S_i = 0, \pm 1$. This model was proposed independently by Blume [14] and Capel [15]. It is a particular case of the Blume-Emery-Griffiths model (BEG) [16]. The BC model has been investigated for years (RG [17], MC [18], TM with FSS [19]) because of its simplicity and a quite complex phase diagram. Especialy the presence of a tricritical point (TCP) attracted much scientific interest. Thus, in spite of the lack of an exact solution, quite much is known about the phase diagram. Our results are in good agreement with the best previous ones.

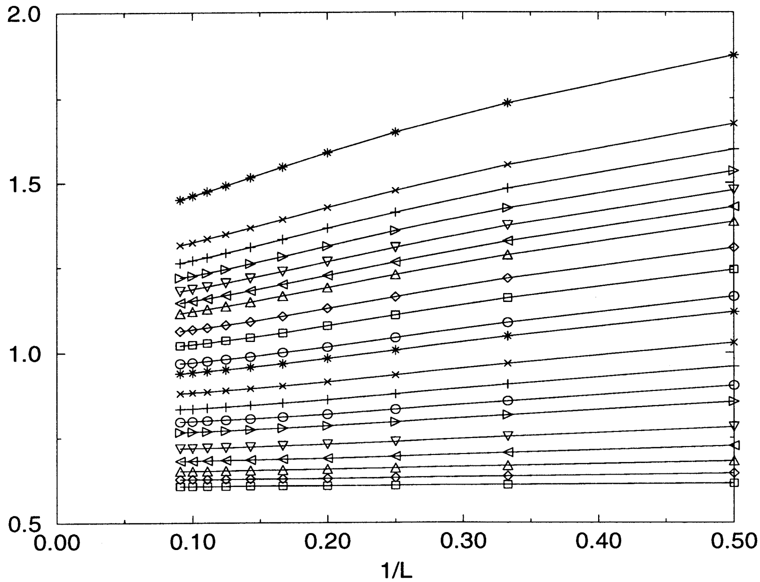

Figure 4: Convergence of the critical coupling constant K_c calculated in different points of the phase diagram of the BC model for finite systems. The upper curves are related to points located closer to TCP.

There are a few differences in our treatment of the AT and BC models. For the BC model we use a scaling relation (3) without a logaritmic term. This results in the absence of a logaritmic term in relation (4) and of course in (5). The maximal system size L for the BC model is equal to 11. There is no exactly known point on the line of second order transitions (as it was in the case of the AT model). Therefore, in order to start our calculations in the same way as we did for the AT model, we assume that the critical point of the $S = 1$ Ising model, obtained in

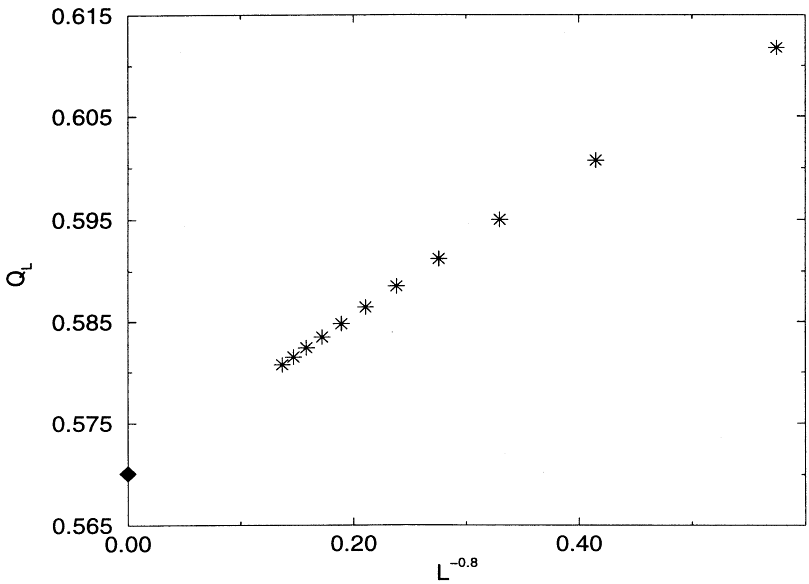

Figure 5: Ratio Q_L (stars) in the critical point of the $q = 3$ Potts model. The filled diamond stands for the extrapolated value.

paper [21], is calculated precisely enough to use this point in a similar way as the exactly known critical point of the $S = \frac{1}{2}$ Ising model was used for the AT model in Section 1.

In this point ($\Delta = 0$) we estimated values of the ratio $Q = \lim_{L\to\infty} Q_L$ for the square ($Q = 0.855 \pm 0.003$) and the rectangular (for the aspect ratio $\alpha = 2$, $Q = 0.809 \pm 0.001$) geometry. These approximate results coincide, as we expected, with those calculated in [12] ($Q = 0.856216 \pm 0.000001$ and $Q = 0.809678 \pm 0.000003$ for the square and the $\alpha = 2$ rectangular geometry respectively).

Our final results for the BC model are presented and compared with other results in Fig. 3.

Fig 4 shows our finite size results. In the vicinity of the tricritical point (TCP) convergence is worse. It is due to crossover phenomena; the TCP belongs to a different universality class. The final results were obtained in the same way as in the case of the AT model. Our accuracy is very good: It changes from about 0% (from our definition in the $S = 1$ Ising point) to 3% in the vicinity of the TCP.

3 q=3 Potts model

The next model that we considered was the $d = 2$, $q = 3$ Potts model on a square lattice ($L \times L$) with reduced hamiltonian:

$$\beta\mathcal{H} = -K \sum_{<i,j>} \delta(\sigma_i, \sigma_j) - H \sum_i \delta(0, \sigma_i), \tag{11}$$

where $\sigma_i = 0, 1, 2$ is a variable at site i and δ is the Kronecker delta. We take $H = 0$. This model exhibits a so called anomalous TCP, which is located in the point ($K = \ln(1 + \sqrt{3})$, $H = 0$) in parameter space [20]. The order parameter for this transition is quite complicated and has the form:

$$M = \frac{qm - L^2}{q - 1}\,, \tag{12}$$

where $m = \sum_i \delta(\sigma_i, 0)$ and $q = 3$ in our case. The ratio Q_L for this model is expressed by formula (2).

We calculated the ratio Q_L in the critical point (anomalous TCP) for different system sizes L ($L \leq 12$) exploiting a transfer matrix technique described above for the AT model. In order to obtain a limiting value $Q = \lim_{L\to\infty} Q_L$ we fitted our results to the same scaling formula like the one used for the BC model, however with different scaling exponents ($y_t = \frac{6}{5}, y_h = \frac{28}{15}$ [20]) and one additional term ($L^{-\frac{4}{5}}$) suggested in paper [21]. In fact this additional term is a leading term what can easily be seen in Fig. 5 where our results are plotted against $L^{-\frac{4}{5}}$.

Linear extrapolations of our data in Fig. 5 allow us to estimate a universal critical point amplitude ratio Q with big accuracy (tab. 1)

number of points	Q_∞	regression error
11	0.5713057	0.0001601435
10	0.5710429	0.0001768326
9	0.5706616	0.0001064718
8	0.5704433	5.984143e-05
7	0.5703282	3.67798e-05
6	0.5702614	2.550278e-05
5	0.5702166	1.908602e-05
4	0.5701832	1.458139e-05
3	0.5701500	—
2	0.5701310	0.0
final estimate	0.5701	0.0001

Table 1: Linear extrapolations (Q_∞) of our results ploted against $L^{-\frac{4}{5}}$ for different number of points. Always the results for the largest systems are used. ($L_{min} = 2$, $L_{max} = 12$)

4 Acknowledgments

The numerical calculations were carried out in the Supercomputing and Networking Center in Poznań on Cray J-916. The work has been supported in part by the Committee for the Scientific Research via grant 2 P302 116 06. We thank also Dr. E. Carlon, Dr. P. Pawlicki and Prof. J. Rogiers for some discussions.

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